

On the ro-vibrational energies for the lithium dimer; maximum-possible rotational levels.

Omar Mustafa*

*Department of Physics, Eastern Mediterranean University,
G. Magusa, north Cyprus, Mersin 10 - Turkey, and
Tel.: +90 392 6301078; fax: +90 3692 365 1604.*

The Deng-Fan potential is used to discuss the reliability of the improved Greene-Aldrich approximation and the factorization recipe of Badawi et al.'s [17] for the central attractive/repulsive core $J(J+1)/2\mu r^2$. The factorization recipe is shown to be a more reliable approximation and is used to obtain the ro-vibrational energies for the $a^3\Sigma_u^+$ - ${}^7\text{Li}_2$ dimer. For each vibrational state only a limited number of the rotational levels are found to be supported by the $a^3\Sigma_u^+$ - ${}^7\text{Li}_2$ dimer.

Keywords: Ro-vibrational energies, Lithium dimer. Maximum-possible rotational levels.

I. INTRODUCTION

The discovery of Bose-Einstein condensation in some ultracold spin-polarized states of the alkali lithium dimer ${}^7\text{Li}_2$ [1] has encouraged intensive experimental as well as theoretical studies on this system [2–7]. Whilst the Bose-Einstein condensation formation in ${}^7\text{Li}_2$ dimer is found to depend on the interaction potential of the lowest triplet excited $a^3\Sigma_u^+$ state, its stability is observed to be sensitive to the binding energy of the least bound vibrational state (among the 11 vibrational states supported by the $a^3\Sigma_u^+$ - ${}^7\text{Li}_2$ potential) [2–4]. Spectral analysis were carried out to determine vibrational and rotational constants and dissociation energy for this dimer [3, 5, 6]. The transition probabilities, moreover, depend on the molecular rotational-vibrational (ro-vibrational, hereinafter) levels. A general analytical closed-form solution for molecular ro-vibrational energies (with sufficient reliable accuracy in a broad range of the rotational and vibrational quantum numbers) would be of great interest in Physics and/or Chemistry, for it would allow substantial simplifications of the derivation of molecular transition probabilities [8]. The ro-vibrational energy levels of the $a^3\Sigma_u^+$ - ${}^7\text{Li}_2$ dimer represent the core of the current work.

In the literature, an empirical diatomic molecular potential energy function, $U(r)$, necessarily and desirably satisfies the conditions (cf., e.g., [9, 10])

$$U(\infty) - U(r_e) = D_e, \quad \left. \frac{dU(r)}{dr} \right|_{r=r_e} = 0, \quad \text{and} \quad \left. \frac{d^2U(r)}{dr^2} \right|_{r=r_e} = K_e = (2\pi c)^2 \mu \omega_e^2. \quad (1)$$

Where D_e is the dissociation energy, r_e is the equilibrium bond length, c is the speed of light, μ is the reduced mass, and ω_e is the equilibrium harmonic oscillator vibrational frequency. The introduction of a fourth condition $U(r_e) = 0$ would only shift the potential by a constant at the equilibrium bond length, but never violates the three conditions above [11–19]. For example, the Schiöberg [15], and the improved (or the shifted by a constant) Manning-Rosen potentials share the Deng-Fan [14] diatomic molecular potential form

$$U(r) = D_e \left[1 - \frac{e^{\alpha r_e} - 1}{e^{\alpha r} - 1} \right]^2. \quad (2)$$

Here α denotes the range of the potential and is obtained using the last condition in (1) to read

$$\alpha = \beta + \frac{1}{r_e} W(-r_e \beta e^{-r_e \beta}); \quad \beta = \sqrt{\frac{K_e}{2D_e}},$$

where β is often called the Morse constant [19] and $W(z)$ is the Lambert function. The vibrational spectra of such a model is exactly solvable and a closed form solution exists in the literature (e.g., [11, 12]). The main challenge lies, however, in dealing with the central attractive/repulsive core $J(J+1)/2\mu r^2$ of the radial spherically symmetric Schrödinger equation

$$-\frac{\hbar^2}{2\mu} \frac{d^2 u_{\nu,J}(r)}{dr^2} + \left[\frac{J(J+1)\hbar^2}{2\mu r^2} + U(r) \right] u_{\nu,J}(r) = E_{\nu,J} u_{\nu,J}(r), \quad (3)$$

*Electronic address: omar.mustafa@emu.edu.tr

with ν denoting the vibrational and J denoting the rotational quantum numbers.

In their attempt to obtain the ro-vibrational spectra for the $a^3\Sigma_u^+ - {}^7\text{Li}_2$ dimer, Liu and coworkers [11] have, very recently, used an improved Manning-Rosen empirical potential energy model (2). However, to deal with the central attractive/repulsive core $J(J+1)/2\mu r^2$ (i.e., the rotational-vibrational coupling) they have used the improved Greene-Aldrich approximation [16]

$$\frac{1}{r^2} \approx \alpha^2 \left(\frac{1}{12} + \frac{e^{\alpha r}}{(e^{\alpha r} - 1)^2} \right), \quad (4)$$

and reported the ro-vibrational energy spectra in a closed analytical form as

$$E_{\nu,J} = D_e + \frac{J(J+1)\hbar^2\alpha^2}{24\mu} - \frac{\hbar^2\alpha^2}{2\mu} \left(\frac{\frac{2\mu}{\hbar^2\alpha^2}D_e(e^{2\alpha r_e} - 1)}{\Lambda} - \frac{\Lambda}{4} \right)^2, \quad (5)$$

with

$$\Lambda = 2\nu + 1 + \sqrt{(1 + 2J)^2 + \frac{8\mu}{\hbar^2\alpha^2}D_e(e^{\alpha r_e} - 1)^2}. \quad (6)$$

but never subjected it to a quantitative brute force numerical test for any $J \neq 0$. At this very point, it is obvious that the asymptotic behavior of $e^{\alpha r}/(e^{\alpha r} - 1)^2$ as $\alpha r \rightarrow 0$ would manifest the necessary improvement of the Greene-Aldrich approximation

$$\frac{1}{r^2} \approx \alpha^2 \left(\frac{e^{\alpha r}}{(e^{\alpha r} - 1)^2} \right)$$

into the Taylor series expansion

$$\frac{e^{\alpha r}}{(e^{\alpha r} - 1)^2} \approx \left(\frac{1}{\alpha^2 r^2} - \frac{1}{12} + O(\alpha^2 r^2) \right),$$

which in turn leads to (4). However, one may wonder as to whether such an approximation is an adequate representation of the rotational-vibrational coupling term. Strictly speaking, if such an approximation sacrifices the accuracy for large rotational quantum number $J > 0$ then one should look for an alternative approach and hope for a better and more adequate representation.

In the current proposal, we suggest Badawi et al.'s [17] factorization recipe

$$\frac{r_e^2}{r^2} = C_0 + \frac{C_1}{e^{\alpha r} - 1} + \frac{C_2}{(e^{\alpha r} - 1)^2}, \quad (7)$$

in section 2, as an alternative approach and report a closed form analytical solution for the ro-vibrational energy levels. Although a variant of algebraic approaches are available in the literature (cf., e.g., Infeld and Hull [20], Wybourne [21], and Iachello and Levine [22, 23]), we recollect (in the same section) the supersymmetric quantization recipe used by Jia et al. [18] to obtain the ro-vibrational energies. Moreover, we subject (in section 3) both approaches (4) and (7) into a quantitative brute force numerical test and compare their accuracy performance with those of Roy [19], who have used a generalized pseudospectral (GPS) method to calculate the ro-vibrational energies for six diatomic molecules. We choose the $O_2(X^3\Sigma_g^-)$ molecule for the sake of comparison. Owing to the fact that only 11 vibrational levels are supported by the $a^3\Sigma_u^+ - {}^7\text{Li}_2$ potential (here the Deng-Fan [14] diatomic molecular potential (2) is just one of the available options and need not be the best one for the ${}^7\text{Li}_2$ dimer), one would intuitively expect similar trends for the rotational levels. We shall see that only a limited number of the rotational levels are supported by the $a^3\Sigma_u^+ - {}^7\text{Li}_2$ potential for each available vibrational state. This is also discussed in section 3. To the best of our knowledge, such a study is not reported elsewhere. Section 4 is devoted for our concluding remarks.

II. RO-VIBRATIONAL ENERGIES AND SUPERSYMMETRIC QUANTIZATION RECIPE

In this section we recollect Jia et al.'s [18] work on the 6-parametric exponential-type one-dimensional potential, where a closed form exact energy eigenvalues are obtained. For the sake of our study here, we use a 4-parametric potential and cast the Deng-Fan [14] diatomic molecular potential (2) as

$$U(r) = P_1 + \frac{P_2}{e^{\alpha r} - 1} + \frac{P_3}{(e^{\alpha r} - 1)^2}, \quad (8)$$

where

$$P_1 = D_e ; \quad P_2 = -2D_e (e^{\alpha r_e} - 1) ; \quad P_3 = D_e (e^{\alpha r_e} - 1)^2. \quad (9)$$

Incorporating (7) and (8) into (3) one would write the effective potential as

$$U_{eff}(r) = \frac{J(J+1)\hbar^2}{2\mu r^2} + U(r) = \tilde{P}_1 + \frac{\tilde{P}_2}{e^{\alpha r} - 1} + \frac{\tilde{P}_3}{(e^{\alpha r} - 1)^2}, \quad (10)$$

with

$$\tilde{P}_1 = P_1 + \gamma C_0 ; \quad \tilde{P}_2 = P_2 + \gamma C_1 ; \quad \tilde{P}_3 = P_3 + \gamma C_2 ; \quad \gamma = \frac{J(J+1)\hbar^2}{2\mu r_e^2}. \quad (11)$$

and the values of the C'_i s are obtained in the following manner. Let $y = \alpha(r - r_e)$ then with $\alpha r = y + u$ and $u = \alpha r_e$ one implies that

$$\frac{r_e^2}{r^2} = \frac{1}{(y/u + 1)^2} \quad \text{and} \quad \frac{r_e^2}{r^2} = C_0 + \frac{C_1}{e^{y+u} - 1} + \frac{C_2}{(e^{y+u} - 1)^2}. \quad (12)$$

Retaining the first three terms of the Taylor's expansion near the equilibrium internuclear distance $y \rightarrow 0$ (i.e., $r \rightarrow r_e$) of both expressions in (12) and equating coefficients of same power of y one obtains

$$C_0 = 1 - \left(\frac{1 - e^{-u}}{u} \right)^2 \left[\frac{4u}{1 - e^{-u}} - (3 + u) \right], \quad (13)$$

$$C_1 = 2(e^u - 1) \left[3 \left(\frac{1 - e^{-u}}{u} \right) - (3 + u) \left(\frac{1 - e^{-u}}{u} \right)^2 \right], \quad (14)$$

$$C_2 = \left(\frac{e^u - 1}{u} \right)^2 (1 - e^{-u})^2 \left[(3 + u) - \frac{2u}{1 - e^{-u}} \right]. \quad (15)$$

Which are in exact accord with those reported in equation (4) of [17].

Under such potential parametric settings, one would use the supersymmetric quantum recipe used by Jia et al.[18] and follow, step-by-step, their procedure for our Schrödinger equation in (3), along with the effective potential in (10). Namely, one should set their $P_4 = P_5 = 0$ and their P_1 , P_3 , and P_2 are our current \tilde{P}_1 , \tilde{P}_3 , and \tilde{P}_2 , respectively. Hereby, we only cast the necessary formulae where our superpotential would read

$$\tilde{W}(r) = -\frac{\hbar}{\sqrt{2\mu}} \left(\tilde{Q}_1 + \frac{\tilde{Q}_2}{e^{\alpha r} - 1} \right), \quad (16)$$

where the one-dimensional ground-state like wave function is given by

$$\psi(r) = N \exp \left(-\frac{\sqrt{2\mu}}{\hbar} \int \tilde{W}(r) dr \right) \quad (17)$$

Which, when substituted in (3) along with (10), would result in

$$\tilde{Q}_2^2 - \alpha \tilde{Q}_2 = \frac{2\mu}{\hbar^2} \tilde{P}_3 \implies \tilde{Q}_2 = \frac{\alpha}{2} \left(1 + \sqrt{1 + \frac{8\mu}{\hbar^2 \alpha^2} \tilde{P}_3} \right) \quad (18)$$

$$2\tilde{Q}_1 \tilde{Q}_2 - \alpha \tilde{Q}_2 = \frac{2\mu}{\hbar^2} \tilde{P}_2 \implies \tilde{Q}_1 = \frac{1}{2\tilde{Q}_2} \left[\frac{2\mu}{\hbar^2} (\tilde{P}_2 - \tilde{P}_3) + \tilde{Q}_2^2 \right] \quad (19)$$

and

$$\tilde{Q}_1^2 = \frac{2\mu}{\hbar^2} (\tilde{P}_1 - E_0) \implies E_0 = \tilde{P}_1 - \frac{\hbar^2}{2\mu} \left(\frac{1}{2\tilde{Q}_2} \left[\frac{2\mu}{\hbar^2} (\tilde{P}_2 - \tilde{P}_3) + \tilde{Q}_2^2 \right] \right)^2. \quad (20)$$

Under such settings, the wave function is

$$\psi(r) = N e^{\tilde{Q}_1 r} \left(\frac{e^{\alpha r} - 1}{e^{\alpha r}} \right)^{\tilde{Q}_2/\alpha} \quad (21)$$

and the corresponding eigenvalues are

$$E_{\nu,J} = \tilde{P}_1 - \frac{\hbar^2 \alpha^2}{2\mu} \left[\frac{\frac{2\mu}{\hbar^2 \alpha^2} (\tilde{P}_3 - \tilde{P}_2)}{-1 - 2\nu - \sqrt{1 + \frac{8\mu}{\hbar^2 \alpha^2} \tilde{P}_3}} - \frac{-1 - 2\nu - \sqrt{1 + \frac{8\mu}{\hbar^2 \alpha^2} \tilde{P}_3}}{4} \right]^2, \quad (22)$$

where

$$\tilde{P}_3 - \tilde{P}_2 = D_e (e^{2\alpha r_e} - 1) + \gamma (C_2 - C_1)$$

and

$$\tilde{P}_3 = D_e (e^{\alpha r_e} - 1)^2 + \gamma C_2$$

Hereby, it should be obvious to notice that this result, in (22), is in exact accord with that of Liu and coworkers [11, 12], in (5) and (6), for $J = 0$ and hence $\gamma = 0$ (i.e., only for the vibrational levels). This is also documented in tables 1-5.

III. RESULTS AND DISCUSSION

In connection with the central attractive/repulsive core $J(J+1)/2\mu r^2$, we now subject the improved Greene-Aldrich approximation [16], in (4), and the Badawi et al.'s [17] factorization recipe, in (7), to a quantitative brute force numerical test. Hereby, we use the $O_2(X^3\Sigma_g^-)$ diatomic spectroscopic molecular parameters $D_e = 42041 cm^{-1}$, $\omega_e = 1580.2 cm^{-1}$, and $r_e = 1.207 \text{ \AA}$ used by Roy [19] and report the results in table 1. In the same table, we show the energy shifts $\Delta_{Liu} = E_{Liu} - E_{Roy}$ and $\Delta_{our} = E_{our} - E_{Roy}$ for Liu et al.'s [11] results, in (5), and for our results, in (22), compared with those of Roy's [19] (GPS), respectively. It is obvious that whilst the ro-vibrational energies reported by Liu [11] dramatically shift from those of Roy [19] (i.e., Δ_{Liu} grows from $\sim 11 cm^{-1}$ for $(\nu, J) = (0, 0)$ to $\sim 177 cm^{-1}$ for $(\nu, J) = (0, 20)$ and from $\sim 151 cm^{-1}$ for $(\nu, J) = (5, 10)$ to $\sim 289 cm^{-1}$ for $(\nu, J) = (5, 20)$) as J increases, our energies remain at an almost constant shift from Roy's results (i.e., $\Delta_{our} \sim 11 cm^{-1}$ for $(\nu, J) = (0, 0)$ to $(\nu, J) = (0, 20)$ and $\Delta_{our} \sim 105 cm^{-1}$ for $(\nu, J) = (5, 10)$ to $(\nu, J) = (5, 20)$). This observation would in turn imply that the factorization recipe (7) of Badawi et al. [17] is more stable and more adequate than that of Greene-Aldrich approximation [16] used by Liu et al. [11]. Of course one should expect such energy shifts because of the different forms of the interaction potentials used. Roy [19] have used Tietz-Hua potential whereas the Deng-Fan [14] is used here and also used by Liu [11]. Nevertheless, the Deng-Fan potential is shown to be equivalent to the improved Manning-Rosen potential [12, 13].

We now safely proceed with our calculations for the ro-vibrational energies using the "reliable" factorization recipe (7) of Badawi et al. [17]. In tables 2,3, and 4 we report the ro-vibrational energy levels for the $a^3\Sigma_u^+ - ^7Li_2$ dimer. Here, we have used the $a^3\Sigma_u^+ - ^7Li_2$ dimer spectroscopic molecular parameters $D_e = 333.690 cm^{-1}$, $\omega_e = 65.130 cm^{-1}$, and $r_e = 4.173 \text{ \AA}$ as used by Liu et al. [11]. In table 3, nevertheless, one observes that the energies are listed up to $J = 10$ for $\nu = 7$. Similar limited numbers of the ro-vibrational energies are also observed in table 4. The binding energy is known to satisfy the condition

$$E_{binding} = E_{\nu,J} - D_e < 0. \quad (23)$$

Therefore, when the energies $E_{\nu,J}$ approach the dissociation energy $D_e = 333.690 cm^{-1}$ they would in fact signal the very existence of a maximum possible rotational quantum number, J_{max} , associated with a corresponding vibrational quantum number, ν . That is, for each of the only available 11 vibrational states there is a maximum possible number of rotational levels for the $a^3\Sigma_u^+ - ^7Li_2$ molecular dimer.

In table 5, we report the feasibly "maximum-possible" ro-vibrational energy levels. For example, we observe that for $\nu = 0$ the "maximum-possible" ro-vibrational energy level is $J_{max} = 34$, for $\nu = 1$ is $J_{max} = 32$, for $\nu = 2$ is $J_{max} = 29$, for $\nu = 3$ is $J_{max} = 26$, and so on J_{max} gradually decreases as ν grows up to the 11th vibrational state where only one rotational level is obtained at $J_{max} = 1$. Of course, in judging on the "maximum-possible" ro-vibrational energy level we have taken into account the stability patterns of our energy shifts discussed above for the $O_2(X^3\Sigma_g^-)$ diatomic

molecule (in table 1) and projected such stability patterns for the $a^3\Sigma_u^+ - {}^7\text{Li}_2$ dimer (by comparing our results for $\nu = 0$ with the RKR (Rydberg-Klein-Rees) ones reported in [11]). We may very clearly observe that the improved Greene-Aldrich approximation [16], in (4), used by Liu et al. [11] ceases to satisfy condition (23) at lower values of the rotational quantum number J (documented in tables 3,4, and 5). Indeed, the the Deng-Fan [14] potential (2) (used here) may not be the best interaction potential to describe the $a^3\Sigma_u^+ - {}^7\text{Li}_2$ molecular dimer. It had, nevertheless, shown intuitive consistency with the common sense contemplation on that each of the only available 11 vibrational states may, very well, accommodate a limited number of rotational states.

IV. CONCLUDING REMARKS

In this study, we have considered the Deng-Fan [14] potential (2) and discussed the reliability of two available approximations for the central attractive/repulsive core $J(J+1)/2\mu r^2$ (i.e., the improved Greene-Aldrich approximation [16], in (4), and the Badawi et al.'s [17] factorization recipe, in (7)). We have studied and analyzed the numerical outcomes of both approximations for $J > 0$ using the $O_2(X^3\Sigma_g^-)$ diatomic molecule and compared the results with those of Roy [19]. As long as the rotational quantum number $J > 0$ (especially for $J \gg 0$) is in point, such a comparison suggested that the factorization recipe (7) of Badawi et al. [17] is more reliable than that of Greene-Aldrich approximation [16] used by Liu et al. [11]. The stability and reliability of which is documented in the almost constant energy shifts Δ_{our} (obtained and listed in table 1). That is, $\Delta_{our} \sim 11\text{ cm}^{-1}$ for $(\nu, J) = (0, 0)$ to $(\nu, J) = (0, 20)$ and $\Delta_{our} \sim 105\text{ cm}^{-1}$ for $(\nu, J) = (5, 10)$ to $(\nu, J) = (5, 20)$, whereas Δ_{Liu} grows up from $\sim 11\text{ cm}^{-1}$ for $(\nu, J) = (0, 0)$ to $\sim 177\text{ cm}^{-1}$ for $(\nu, J) = (0, 20)$ and from $\sim 151\text{ cm}^{-1}$ for $(\nu, J) = (5, 10)$ to $\sim 289\text{ cm}^{-1}$ for $(\nu, J) = (5, 20)$.

On the other hand, we have used the same potential to study the ro-vibrational energies for the $a^3\Sigma_u^+ - {}^7\text{Li}_2$ molecular dimer. We have shown that only a limited number of the rotational levels is supported by the $a^3\Sigma_u^+ - {}^7\text{Li}_2$ dimer. That is, the $\nu = 0$ vibrational state accommodates only 34 rotational levels, $\nu = 1$ accommodates 32, $\nu = 2$ accommodates 29, $\nu = 3$ accommodates 26, $\nu = 4$ accommodates 23, $\nu = 5$ accommodates 20, $\nu = 6$ accommodates 16, $\nu = 7$ accommodates 11, $\nu = 8$ accommodates 9, $\nu = 9$ accommodates 5, and $\nu = 10$ accommodates only one rotational level. To the best of our knowledge, this has never been reported elsewhere.

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Table 1:

ν	J	Ref. [11]	Eq.(22)	GPS [19]	Δ_{Liu}	Δ_{our}
0	0	786.380	786.380	775.074	11.306	11.306
	1	789.941	789.153	777.848	11.562	11.305
	2	797.066	794.699	783.395	13.671	11.304
	10	982.257	938.844	927.562	54.695	11.282
	15	1213.661	1118.890	1107.634	106.027	11.256
	20	1533.912	1367.943	1356.714	177.198	11.229
5	10	8412.365	8366.286	8261.257	151.108	105.029
	15	8635.437	8534.849	8429.967	205.470	104.882
	20	8944.154	8768.000	8663.303	280.851	104.679

Table 2

ν	J	Ref.[11]	Eq.(22)	RKR [11]	ν	J	Ref.[11]	Eq.(22)	RKR [11]
0	0	31.7694	31.7694	31.857	2	0	142.3939	142.3939	142.523
	1	32.4900	32.3035			1	143.0660	142.8583	
	2	33.9311	33.3714			2	144.4101	143.7867	
	3	36.0919	34.9720			3	146.4255	145.1782	
	4	38.9717	37.1038			4	149.1115	147.0311	
	5	42.5692	39.7651			5	152.4668	149.3436	
	10	71.2648	60.9108			10	179.2270	167.6973	
	15	117.5735	94.7215			15	222.4000	196.9618	
1	0	90.3292	90.3292	90.453	3	0	188.0375	188.0375	188.240
	1	91.0254	90.8283			1	188.6858	188.4676	
	2	92.4177	91.8260			2	189.9822	189.3274	
	3	94.5054	93.3215			3	191.9262	190.6159	
	4	97.2877	95.3132			4	194.5168	192.3315	
	5	100.7635	97.7991			5	197.7531	194.4724	
	10	128.4858	117.5415			10	223.5620	211.4519	
	15	173.2177	149.0671			15	265.1939	238.4792	

Table 3

ν	J	Ref. [11]	Eq.(22)	RKR [11]	ν	J	Ref. [11]	Eq.(22)	RKR [11]
4	0	227.332	227.332	227.679	6	0	287.160	287.160	287.665
	1	227.9573	227.7287			1	287.7389	287.4898	
	2	229.2066	228.5206			2	288.8955	288.1480	
	3	231.0799	229.7072			3	290.6299	289.1341	
	4	233.5763	231.2870			4	292.9411	290.4465	
	5	236.6949	233.2580			5	295.8281	292.0833	
	10	261.5633	248.8779			10	318.8468	305.0266	
	15	301.6712	273.6914			15	355.9576	325.4829	
5	0	260.350	260.350	260.837	7	0	307.832	307.832	308.098
	1	260.9517	260.7128			1	308.3877	308.1285	
	2	262.1544	261.4374			2	309.4988	308.7209	
	3	263.9578	262.5233			3	311.1647	309.6083	
	4	266.3611	263.9687			4	313.3849	310.7892	
	5	269.3633	265.7717			5	316.1581	312.2614	
	10	293.3016	280.0462			10	338.2671	323.8878	
	15	331.9027	302.6694						

Table 4

ν	J	Ref.[11]	Eq.(22)	RKR [11]
8	0	322.432	322.432	322.155
	1	322.9654	322.6962	
	2	324.0314	323.2236	
	3	325.6298	324.0134	
	4	327.7599	325.0640	
	5	330.4205	326.3735	
	6	333.6105	327.9394	
	7	337.3283	329.7585	
9	8	341.5722	331.8272	
	0	331.027	331.027	330.170
	1	331.5383	331.2592	
	2	332.5598	331.7222	
	3	334.0913	332.4154	
10	4	336.1322	333.3373	
	0	333.683	333.683	333.269

Table 5

ν	J	Ref.[11]	Eq.(22)	ν	J	Ref.[11]	Eq.(22)
0	20	181.0396	140.3931	4	20	356.5889	306.8700
	25	261.0387	196.7792		23	396.4097	330.3157
	30	356.7841	262.3569	5	20	384.7428	332.8067
	34	444.0906	320.1449		16	365.0368	330.4078
1	20	234.5100	191.5654	7	11	344.3232	327.0375
	25	311.7476	243.8808		9	346.3401	334.1416
	30	404.1552	304.4789	9	5	338.6815	334.4858
	32	445.1631	330.6137		10	334.1715	333.8826
2	20	281.5434	236.3203				
	25	356.0508	284.6083				
	29	426.2105	328.6431				
3	20	322.2125	274.7310				
	25	394.0204	319.0345				
	26	410.0931	328.7317				

Tables captions:

Table 1: Ro-vibrational energies $E_{\nu,J}$ (in cm^{-1} units) for $O_2(X^3\Sigma_g^-)$, where Δ_{Liu} and Δ_{our} denote the energy shifts for Liu et al's [11] in Eq.(5) and our results from Eq.(22) compared with those of Roy's [19] (GPS), respectively.

Table 2: Ro-vibrational energies $E_{\nu,J}$ (in cm^{-1} units) for $^7Li_2(a^3\Sigma_u^+)$ with $\nu = 0, 1, 2$, and 3. Our results from Eq.(22) are compared with those of Liu et al's [11] in Eq.(5) and those of RKR [11] whenever possible.

Table 3: Ro-vibrational energies $E_{\nu,J}$ (in cm^{-1} units) for $^7Li_2(a^3\Sigma_u^+)$ with $\nu = 4, 5, 6$, and 7. Our results from Eq.(22) are compared with those of Liu et al's [11] in Eq.(5) and those of RKR [11] whenever possible.

Table 4: Ro-vibrational energies $E_{\nu,J}$ (in cm^{-1} units) for $^7Li_2(a^3\Sigma_u^+)$ with $\nu = 8, 9$ and 10. Our results from Eq.(22) are compared with those of Liu et al's [11] in Eq.(5) and those of RKR [11] whenever possible.

Table 5: Ro-vibrational energies $E_{\nu,J}$ (in cm^{-1} units) for $^7Li_2(a^3\Sigma_u^+)$. Our results from Eq.(22) are compared with those of Liu et al's [11] in Eq.(5). For each value of ν we show the "maximum-possible" rotational quantum number J (i.e., J_{max} is the last value of J for each ν).